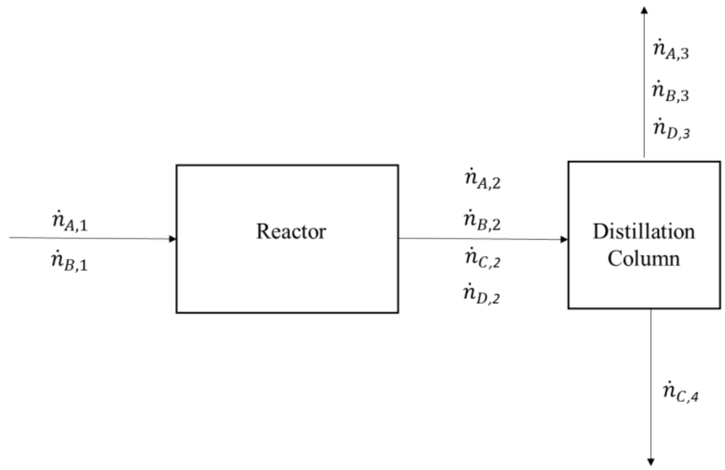
Chemical Engineering 140 **April 5, 2021**

Midterm 2 Solutions

Problem 1



First, find the composition of stream 2. Write the mole balances of species *A*, *B*, *C*, and *D* in terms of extent of reaction (ξ_1 and ξ_2).

$$\dot{n}_{A,2} = \dot{n}_{A,1} - \xi_1 - 2\xi_2 \quad (1)$$
$$\dot{n}_{A,2} = 50 - 30 - 2(5) = 10\ mol/s \quad (2)$$

$$\dot{n}_{B,2} = \dot{n}_{B,1} - \xi_1 - \xi_2 \quad (3)$$
$$\dot{n}_{B,2} = 50 - 30 - 5 = 15\ mol/s \quad (4)$$

$$\dot{n}_{C,2} = \dot{n}_{C,1} + 2\xi_1 \quad (5)$$
$$\dot{n}_{C,2} = 0 + 2(30) = 60\ mol/s \quad (6)$$

$$\dot{n}_{D,2} = \dot{n}_{D,1} + 3\xi_2 \quad (7)$$
$$\dot{n}_{D,2} = 0 + 3(5) = 15\ mol/s \quad (8)$$

All of species A, B, and D exits through stream 3. The total moles in stream 3 must be:

$$\dot{n}_3 = 10 + 15 + 15 = 40\ mol/s \quad (9)$$

The composition of stream is then:

$$y_{A,3} = \frac{10}{40} = \mathbf{0.25} \quad (10)$$
$$y_{B,3} = \frac{15}{40} = \mathbf{0.375} \quad (11)$$
$$y_{D,3} = \frac{15}{40} = \mathbf{0.375} \quad (12)$$

Problem 2

a. Heat of reaction is positive, so the reaction is endothermic. If the temperature of the reaction increases, the forward reaction will be favored.

b. K_{eq} is defined as $K_{eq}(T) = \prod_i (y_i P)^{\nu_i}$. If the forward reaction is favored, K_{eq} will increase.

This can be proved by calculating K_{eq} at T = 400K using the following thermodynamic relationship:

$$\ln\left(\frac{K_{eq}(T)}{K_{eq}(T_0)}\right) = \frac{-\Delta H^0_{rxn}}{R}\left[\frac{1}{T} - \frac{1}{T_0}\right] \tag{1}$$

$$\ln\left(\frac{K_{eq}(T)}{4}\right) = \frac{\left(-\frac{15kJ}{mol}\right)\left(\frac{1000J}{mol}\right)}{\left(\frac{8.314J}{K * mol}\right)}\left[\frac{1}{400K} - \frac{1}{300K}\right] \tag{2}$$

$$\ln\left(\frac{K_{eq}(T)}{4}\right) = 1.503 \tag{3}$$

$$K_{eq}(T) = 17.98 \tag{4}$$

c. Using conversion of species A, X_A, the moles of each species can be calculated:

$$n_{A,2} = n_{A,1} - n_{A,1}X_A = n_{A,1}(1 - X_A) \tag{5}$$

$$n_{B,2} = n_{B,1} - n_{A,1}X_A \tag{6}$$

We know A and B are equimolar in the inlet stream, so $n_{B,1} = n_{A,1}$

$$n_{B,2} = n_{A,1} - n_{A,1}X_A = n_{A,1}(1 - X_A) \tag{7}$$

$$n_{C,2} = n_{C,1} + 2n_{A,1}X_A \tag{8}$$

$$n_{C,2} = 2n_{A,1}X_A \tag{9}$$

Sum over all species to determine total moles in stream 2:

$$n_2 = 2n_{A,1} \tag{10}$$

Now, determine the mole fractions of each species in stream 2 as a function of conversion of species A:

$$y_{A,2} = \frac{n_{A,1}(1 - X_A)}{2n_{A,1}} = \frac{1}{2}(1 - X_A) \tag{11}$$

$$y_{B,2} = \frac{n_{A,1}(1 - X_A)}{2n_{A,1}} = \frac{1}{2}(1 - X_A) \tag{12}$$

$$y_{C,2} = \frac{2n_{A,1}X_A}{2n_{A,1}} = X_A \tag{13}$$

Using the ideal gas law, the given rate law can be rewritten in the following form:

$$r_A = -k\left(\frac{P}{RT}\right)^2\left(y_A y_B - \frac{1}{K_{eq}} y_C^2\right) \tag{14}$$

Substitute equations 11-13 into equation 14 to get an equation in terms of conversion:

$$r_A = -k\left(\frac{P}{RT}\right)^2\left(\frac{1}{4}(1 - X_A)^2 - \frac{1}{K_{eq}} X_A^2\right) \tag{15}$$

d. The governing equation for a PFR is:

$$\frac{dX_A}{dV} = \frac{-r_A}{n_{A,1}} \tag{16}$$

$$\int_0^V dV = \int_0^{X_A} \frac{n_{A,1}}{-r_A} dX_A \tag{17}$$

$$\int_0^V dV = \frac{n_{A,1}}{k}\left(\frac{RT}{P}\right)^2 \int_0^{X_A} \frac{1}{\left(\frac{1}{4}(1 - X_A)^2 - \frac{1}{K_{eq}} X_A^2\right)} dX_A \tag{18}$$

e. Before integrating, substitute the value of K_{eq} into the rate law since this will greatly simplify integration:

$$\int_0^V dV = \frac{n_{A,1}}{k}\left(\frac{RT}{P}\right)^2 \int_0^{X_A} \frac{1}{\left(\frac{1}{4}(1 - X_A)^2 - \frac{1}{4} X_A^2\right)} dX_A \tag{19}$$

$$V = \frac{n_{A,1}}{k}\left(\frac{RT}{P}\right)^2 [-2\ln(1 - 2X_A)|_0^{0.3} \tag{20}$$

$$V = \frac{n_{A,1}}{k}\left(\frac{RT}{P}\right)^2 (1.832) \tag{21}$$

$$V = 77.1L \tag{22}$$

f.

i. What is the molar flow rate of stream 2?
1400 mol/s

ii. What is the recycle ratio?
400/1000 = 0.4

iii. What is the composition of stream 3?

$$y_{A,2} = \frac{n_{A,1}(1 - X_A)}{2n_{A,1}} = \frac{1}{2}(1 - X_A) = 0.35 \tag{11}$$

$$y_{B,2} = \frac{n_{A,1}(1 - X_A)}{2n_{A,1}} = \frac{1}{2}(1 - X_A) = 0.35 \tag{12}$$

$$y_{C,2} = \frac{2n_{A,1}X_A}{2n_{A,1}} = X_A = 0.3 \tag{13}$$

iv. What is the overall conversion of species A?

$$X_{A,\text{overall}} = 0.42$$